L-Proline, N-octanoyl-, heptadecyl ester

Inchi: InChI=1S/C30H57NO3/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-20-22-27-34-30(33)28-24
InchiKey: VJMUHNZYVBDTTE-UHFFFAOYSA-N
Formula: C30H57NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCCCC
Mol. weight [g/mol]: 479.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.59		Crippen Method
logp	8.753		Crippen Method
mcvol	441.690	ml/mol	McGowan Method
rinpol	3567.00		NIST Webbook
rinpol	3567.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346250&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.